Focus on Informatics

This *JASMS* Focus section on Informatics includes four papers that demonstrate the range of problems that can be addressed by employing mathematics in combination with mass spectrometry. While many of the oral presentations at the January, 2001 Sanibel Meeting (reviewed in *JASMS* **2001**, *12*, 475–477) were tutorial in nature, these papers exemplify four applications of informatics to problems in mass spectrometry. In this context it is important to keep in mind a slide by Barry Wise in his tutorial lecture on chemometrics. He defined chemometrics as a discipline that uses mathematical and statistical methods to relate measurements to the state of a system by designing or selecting optimal measurement procedures and experiments. He made the further point that such approaches are not the application of a fixed set of mathematical procedures of any given type. We feel that these four examples are true to his definitions and that the breadth of the applications covered by them is illustrative of the range and power of such techniques.

The paper of Seto et al. uses a variation of one of the classical techniques of informatics, experimental design, to optimize an LC-MS procedure. Because the authors' approach is so conceptually accessible, this paper may spur others to use these kinds of methods in the design of their own analyses.

Harrington and his colleagues describe the use of neural networks for identification of bacteria. It is an application of a powerful chemometrics approach to the solution of a complex problem. While on the one hand this paper represents the latest in a long series of applications of chemometrics to bacterial classification using pyrolysis mass spectrometry, the speed and reliability of the authors' approach represents an important advance. One looks forward to the application of such approaches to the characterization of protein mixtures produced in MALDI spectra which are currently being advocated as clinical diagnostic tools (*Nat. Rev. Genet.* **2000**, *1*, 48–56).

Parker's paper presents a novel approach to using the information in a MALDI peptide map. Current methods of protein identification from such data are based totally on searching data bases using mass information alone. For the first time, Parker incorporates chemical information about the peptides to predict ion intensities and thereby is successful in extracting more protein identifications from a data set than would be possible using conventional methods.

The paper by Blank et al. illustrates the use of a well known non-parametric statistic to characterize the mass spectra of intact proteins. This type of approach may be of value in recognizing the presence of microheterogeneity in proteins—an issue of potential concern to manufacturers of recombinant molecules.

We hope that you find these papers to be stimulating and provocative to your own research.

Alfred L. Yergey
Guest Editor

Veronica M. Bierbaum
Associate Editor

Published online November 19, 2001

1044-0305/02/$20.00
PII S1044-0305(01)00340-3
(J Am Soc Mass Spectrom 2002, 13, 1)